S-Hydroxymethylthiobenzoate

Inchi: InChI=1S/C8H8O2S/c9-6-11-8(10)7-4-2-1-3-5-7/h1-5,9H,6H2
InchiKey: MNTZJQAAOYSCMM-UHFFFAOYSA-N
Formula: C8H8O2S
SMILES: O=C(SCO)c1ccccc1
Mol. weight [g/mol]: 168.22

Physical Properties

Property code	Value	Unit	Source
af	0.6086		Cheméo Relay (1.0)
gf	-103.73	kJ/mol	Joback Method
hf	-245.91	kJ/mol	Cheméo Relay (1.0)
hfus	20.33	kJ/mol	Joback Method
hvap	87.88	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-1.87		Cheméo Relay (1.0)
logp	1.510		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	560.25	K	Cheméo Relay (1.0)
tc	810.51	K	Cheméo Relay (1.0)
tf	336.28	K	Cheméo Relay (1.0)
vc	0.418	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.41	J/mol×K	623.95	Joback Method
cpg	289.94	J/mol×K	661.26	Joback Method
cpg	298.78	J/mol×K	698.56	Joback Method
cpg	306.95	J/mol×K	735.87	Joback Method
cpg	314.47	J/mol×K	773.17	Joback Method
cpg	321.37	J/mol×K	810.48	Joback Method
cpg	327.68	J/mol×K	847.78	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23853330&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume